The Cone of Positive Generalized Matrix Functions

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ABSTRACT

Let $c : \mathrm{S}_n \to \mathbb{C}$ be a complex-valued function on the symmetric group S_n, and let $A = (a_{ij})$ be an n-by$n$ complex matrix. The determinant-like polynomial

$$d(c, A) = \sum_{\sigma} c(\sigma) \prod_{t=1}^{n} a_{t\sigma(t)}$$

in the n^2 entries of A is called a *generalized matrix function*. The restriction of $d(c, \cdot)$ to hermitian matrices $(a_{ij} = \bar{a}_{ji})$ is a nonlinear hermitian form in the $(n^2 + n)/2$ complex entries a_{ij}, with $i \leqslant j$. In this paper we examine the cone $\mathbf{C}_n$ of functions c satisfying the inequality $0 \leqslant d(c, A)$ for all hermitian matrices A. For $n = 4$ (the smallest nontrivial case), we give a complete description of $\mathbf{C}_4$ and its extreme rays. If c is a function in $\mathbf{C}_4$, then $d(c, A)$ is a sum of squares of the absolute values of nonlinear hermitian forms in the a_{ij}. For $n \geqslant 6$, we exhibit a family of extreme rays in $\mathbf{C}_n$. For each c (not necessarily in $\mathbf{C}_n$), we define a square matrix $M(c)$ and show that if the comparison matrix of $M(c)$ is positive semidefinite, then c is in $\mathbf{C}_n$.

INTRODUCTION

Each complex-valued function $c : \mathrm{S}_n \to \mathbb{C}$ defined on the symmetric group of permutations S_n gives rise to a *generalized matrix function* $d(c, \cdot)$ defined on the n-by-n matrices $A = (a_{ij})$ by

$$d(c, A) = \sum_{\sigma \in \mathrm{S}_n} c(\sigma) \prod_{t=1}^{n} a_{t\sigma(t)}.$$

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The best-known generalized matrix function is the determinant, which comes from the choice $c(\sigma) = \pm 1$—depending on the sign of σ. In this paper, we are interested in *positive* generalized matrix functions: those for which

$$d(c, A) \geqslant 0$$

for all A in the set H_n of n-by$n$ hermitian matrices. In this case we also say that the function c is *positive.*

The determinant is not a positive generalized matrix function, so before going on we give two examples of generalized matrix functions that are positive.

EXAMPLE 1. Define c on S_4 by $c((12)(34)) = 1$ and $c(\sigma) = 0$ for all other permutations σ in S_4. Then $d(c, A) = a_{12}a_{21}a_{34}a_{43} = |a_{12}|^2|a_{34}|^2 \geqslant 0$ for all $A(a_{ij})$ in H_4.

The next example is only a little more complicated.

EXAMPLE 2. Let α be a complex number, and define c on S_4 by

$$c((12)(34)) = 1, \qquad c((1234)) = \alpha,$$

$$c((1432)) = \bar{\alpha}, \qquad c((23)(41)) = |\alpha|^2,$$

and $c(\sigma) = 0$ for all other permutations σ in S_4. Then for $A = (a_{ij})$ in H_4,

$$\begin{aligned} d(c, A) &= a_{12}a_{34}a_{21}a_{43} + \alpha a_{12}a_{34}a_{23}a_{41} \\ &\qquad + \bar{\alpha}a_{32}a_{14}a_{21}a_{43} + |\alpha|^2 a_{32}a_{14}a_{23}a_{41} \\ &= |a_{12}a_{34} + \overline{\alpha a_{23}a_{41}}|^2 \geqslant 0. \end{aligned}$$

Of course, Example 1 is just a special case of Example 2 in which $\alpha = 0$.

Since $d(c,\cdot)$ is linear in c, the set

$$\mathbf{C}_n = \{c : c \text{ is positive}\}$$

is a convex cone. The purpose of this paper is to study the structure of $\mathbf{C}_n$.

A great deal of attention has been paid to a related class of functions on S_n—namely, those c for which $d(c, A) \geqslant 0$ for all positive semidefinite hermitian matrices A. These functions form a cone $\mathbf{W}_n$, which contains $\mathbf{C}_n$. Very little is known about the structure of $\mathbf{W}_n$, but [1] contains some information about the dual cone and extreme rays in $\mathbf{W}_n$. The outstanding conjecture about $\mathbf{W}_n$ is this: if c is an irreducible character on S_n of degree r and $\chi \equiv 1$ is the principal character on S_n, then $r\chi - c \in \mathbf{W}_n$. Restated in terms of generalized matrix functions, this conjecture is equivalent to the permanental dominance conjecture: $d(c, A) \leqslant r \operatorname{per} A$, for all positive semidefinite hermitian matrices A. (Here, per stands for the permanent—the generalized matrix function corresponding to the principle character $c \equiv 1$.) For a good survey of the results surrounding this conjecture see Merris [2]. Now we return to the study of the cone $\mathbf{C}_n$.

EXTREME RAYS

The *ray* generated by an element $c \in \mathbf{C}_n$ consists of all nonnegative multiples of c and is denoted by

$$\langle c \rangle = \{rc : r \geqslant 0\}.$$

The ray $\langle c \rangle$ is *extreme* if it is not possible to write $c = c_1 + c_2$, with $c_1, c_2 \in \mathbf{C}_n$, except in the trivial way in which $c_1, c_2 \in \langle c \rangle$.

An inequality of the type $0 \leqslant d(c, A)$ for all $A \in H_n$ cannot be improved if c is an extreme ray. More precisely, if $\langle c \rangle$ is an extreme ray and $0 \leqslant d(b, A) \leqslant d(c, A)$ for all $A \in H_n$, then both b and $c - b$ are in $\mathbf{C}_n$. Now since $\langle c \rangle$ is an extreme ray and $b + (c - b) = c$, we have $b \in \langle c \rangle$, and it follows that $b = rc$ for some $0 \leqslant r \leqslant 1$. In an effort to understand the nature of inequalities of the form $0 \leqslant d(c, A)$, for all $A \in H_n$, we shall describe a class of extreme rays in $\mathbf{C}_n$. For $n = 4$—the least nontrivial case —we shall describe *all* extreme rays in $\mathbf{C}_4$. (The rays generated by the functions c in Example 2 are extreme rays in $\mathbf{C}_4$.)

SPARSE FUNCTIONS

To describe the sparse functions in $\mathbf{C}_n$, we begin with an arbitrary complex number $\alpha \neq 0$ and a permutation μ in S_n, each of whose disjoint cycles has even length. (Of course, such a permutation μ exists only if n is even. But, as we shall see later, $C_n = \{0\}$ if n is odd.) So suppose the disjoint cycle decomposition of μ is

$$\mu = \mu_1 \mu_2 \cdots \mu_r, \tag{1}$$

where

$$\mu_s = (i(s,1), i(s,2), \cdots, i(s,l_s)), \tag{2}$$

in which l_s, the length of the cycle μ_s, is even, and $i(s, 1)$ is the least integer in the orbit of μ associated with μ_s.

If each cycle μ_s is a transposition, then define the *sparse function* c corresponding to μ by $c(\mu) = 1$, and $c(\sigma) = 0$ for all $\sigma \neq \mu$. If some cycle μ_s has length greater than two, then define the *sparse function* c corresponding to μ and α to be nonzero on only four permutations. Two of them are μ and μ^{-1}, and the values of c at these permutations are given by

$$c(\mu) = \alpha, \qquad c(\mu^{-1}) = \bar{\alpha}. \tag{3}$$

Each of the other two permutations τ, δ at which c is nonzero is a product of disjoint transpositions:

$$\begin{aligned} \tau &= \prod_{s=1}^{r} (i(s,1), i(s,2))(i(s,3), i(s,4)) \cdots (i(s,l_s - 1), i(s,l_s)), \\ \delta &= \prod_{s=1}^{r} (i(s,2), i(s,3)) \cdots (i(s,l_s - 2), i(s,l_s - 1))(i(s,l_s), i(s,1)). \end{aligned} \tag{4}$$

Define

$$c(\tau) = 1 \quad \text{and} \quad c(\delta) = |\alpha|^2. \tag{5}$$

This completes the description of the sparse function c corresponding to μ and α. Now we can state the main results about extreme rays in $\mathbf{C}_n$.

THEOREM 3. *Let n be even, and let c be the sparse function corresponding to a complex number α and a permutation μ, all of whose cycles have even length. Then*

(i) *$c \in \mathbf{C}_n$, and*

(ii) *c generates an extreme ray of $\mathbf{C}_n$ whenever μ has at most one cycle of length greater than two.*

The converse of Theorem 3(ii) is false. Using a tedious argument, one can show that the sparse function in $\mathbf{C}_8$ corresponding to $\mu = (1234)(5678)$ and $\alpha = 1$ generates an extreme ray even though μ has more than one cycle of length greater than two. (This function, c, appears in Example 6.) But for $n = 6$, every permutation μ whose cycle lengths are even is either a 6-cycle, a product of a 2-cycle and a 4-cycle, or a product of three 2-cycles. Thus μ has at most one cycle of length greater than 2, and it follows from Theorem 3 that every sparse function in $\mathbf{C}_6$ generates an extreme ray. Similarly, every sparse function in $\mathbf{C}_4$ generates an extreme ray. But in $\mathbf{C}_4$ every extreme ray is generated by a sparse function. In fact, more is true.

THEOREM 4. *Every function in $\mathbf{C}_4$ is a nonnegative linear combination of sparse functions.*

CONJUGATES

Some extreme rays are not generated by a sparse function. Let $c : \mathrm{S}_n \to \mathbb{C}$ be a function on S_n, and let ϕ be a permutation in S_n. The *conjugate* of c with respect to ϕ is the function $b : \mathrm{S}_n \to \mathbb{C}$ defined by

$$b(\sigma) = c(\phi^{-1}\sigma\phi) \tag{6}$$

for all σ in S_n. The generalized matrix functions $d(c, \cdot)$ and $d(b, \cdot)$ are related in the following way:

$$d(c, P^TAP) = d(b, A), \tag{7}$$

where P is the permutation matrix corresponding to the permutation ϕ. To see this, denote the diagonal product of the matrix A corresponding to σ by

$$\Pi(\sigma, A) = \prod_{t=1}^{n} a_{t\sigma(t)}.$$

Then $\Pi(\sigma, P^TAP) = \Pi(\phi\sigma\phi^{-1}, A)$, from which (7) follows.

Now since $P^TAP \in H_n$ if and only if $A \in H_n$, it is easy to prove that the conjugate of a positive function is positive and that the conjugate of an extreme ray is an extreme ray.

THEOREM 5. *Let $c : S_n \to \mathbb{C}$ be a function on S_n, and let b be a conjugate of c. Then*

(i) *$c \in \mathbf{C}_n$ if and only if $b \in \mathbf{C}_n$, and*

(ii) *$\langle c \rangle$ is an extreme ray in $\mathbf{C}_n$ if and only if $\langle b \rangle$ is an extreme ray in $\mathbf{C}_n$.*

The conjugate of a sparse function, however, need not be sparse.

EXAMPLE 6. Let $c \in \mathbf{C}_n$ be the sparse function corresponding to $\mu = (1234)(5678)$ and the complex number α. Then the permutations defined in (4) are

$$\tau = (12)(34)(56)(78) \quad \text{and} \quad \delta = (23)(14)(67)(58),$$

and the only nonzero values of c are given by $c(\tau) = 1$, $c(\mu) = \alpha$, $c(\mu^{-1}) = \bar{\alpha}$, and $c(\delta) = |\alpha|^2$.

The conjugate b or c corresponding to the permutation $\phi = (58)(67)$ attains nonzero values as follows:

$$1 = c(\tau) = b(\phi\tau\phi^{-1}) = b((12)(34)(56)(78)),$$

$$\alpha = c(\mu) = b(\phi\mu\phi^{-1}) = b((1234)(5876)),$$

$$\bar{\alpha} = c(\mu^{-1}) = b(\phi\mu^{-1}\phi^{-1}) = b((1432)(5678)),$$

$$|\alpha|^2 = c(\delta) = b(\phi\delta\phi^{-1}) = b((23)(14)(67)(58)).$$

But b is not a sparse function. The sparse function corresponding to $\phi\mu\phi^{-1}$ is nonzero on (1234)(5876), (1432)(5678), (12)(34)(58)(76), and (23)(41)(87)(65); the sparse function corresponding to $\phi\mu^{-1}\phi^{-1}$ is nonzero on (1432)(5678), (1234)(5876), (14)(32)(56)(78), and (43)(21)(67)(85). Neither of these sparse functions is equal to b.

TENSOR PRODUCTS

In this section we describe a way to construct a function $c \in \mathbf{C}_n$ from two functions $c_1 \in \mathbf{C}_p$ and $c_2 \in \mathbf{C}_q$, where $p + q = n$. Let

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$$

be in H_n, where $A_{11} \in H_p$ and $A_{22} \in H_q$. Clearly $d(c_1, A_{11})d(c_2, A_{22}) \geqslant 0$, and we can define a function $c = c_1 \otimes c_2 \in \mathbf{C}_n$ such that $d(c, A) = d(c_1, A_{11})d(c_2, A_{22})$ as follows:

$$c((\theta, \pi)) = c_1(\theta)c_2(\pi) \qquad \text{if} \quad (\theta, \pi) \in \mathrm{S}_p \times \mathrm{S}_q,$$

$$c(\sigma) = 0 \qquad \text{if} \quad \sigma \notin \mathrm{S}_p \times \mathrm{S}_q.$$

Here, $\mathrm{S}_p \times \mathrm{S}_q$ is embedded in S_n in the usual way.

THEOREM 7. *Let $c_1 \in \mathbf{C}_p$ and $c_2 \in \mathbf{C}_q$. Then*

(i) *$c_1 \otimes c_2 \in \mathbf{C}_{p+q}$, and*

(ii) *if c_1 and c_2 are nonzero, then $c_1 \otimes c_2$ generates an extreme ray in $\mathbf{C}_{p+q}$ if and only if c_1 and c_2 generate extreme rays in $\mathbf{C}_p$ and $\mathbf{C}_q$.*

Every extreme ray in $\mathbf{C}_n$ of which I am aware either is generated by a sparse function or a conjugate of a sparse function or is a tensor product $c_1 \otimes c_2 \otimes \cdots \otimes c_k$ of sparse functions and conjugates of sparse functions. But I suspect there are others.

THE MATRIX $M(c)$

The inequality $0 \leqslant d(c, A)$ for all $A \in H_n$ imposes very strong conditions on the complex-valued function c. In particular, the values of c are mostly zero.

LEMMA 8. *If $c \in \mathbf{C}_n$ and σ is a permutation in S_n with a cycle of odd length, then $c(\sigma) = 0$.*

Now unless n is even, every permutation in S_n has an odd cycle. It follows from Lemma 8 that $\mathbf{C}_n = \{0\}$ if n is odd. So from here on we will assume that $n = 2k$ is even and that E_n stands for the subset of permutations in S_n all of whose cycles have even length. (None of the permutations in E_n has a fixed point, because a fixed point is a cycle of length one, which is odd.) Since, by Lemma 8, each function $c \in \mathbf{C}_n$ is nonzero only on E_n, we will henceforth consider only the functions c from E_n to $\mathbb{C}$.

The main idea in this section is to take a function $c : E_n \to \mathbb{C}$ and arrange its values in a square matrix $M(c)$. The nature of the matrix $M(c)$ will in some cases determine whether c is in $\mathbf{C}_n$. Of course, in order to have any chance of using the values $c(\sigma)$ for $\sigma \in E_n$ as the entries of a square matrix, $|E_n|$ must be a perfect square. In fact $|E_n| = N^2$, where $N = 1 \times 3 \times \cdots \times$

$(2k-1)$. (Remember that $n = 2k$.) A more general combinatorial result is proved in [4] using generating functions. But it suits our purpose here to show that $|E_n| = N^2$ by revisiting the construction of the sparse functions.

In the construction of a sparse function, we begin with a permutation μ in E_n, which is a product of the disjoint cycles given in (1) and (2). The permutation μ gives rise to two new permutations τ, δ defined in (4). Both τ and δ are in the subset P_n of E_n consisting of permutations all of whose cycles have length two. In other words, P_n is the conjugate class of S_n consisting of the involutions with no fixed points. So we have a correspondence from E_n to $P_n \times P_n$ given by $\mu \to (\tau, \delta)$. This correspondence is a bijection, which (since $|P_n| = N$) shows that $|E_n| = N^2$.

We prove later that the map $\mu \to (\tau, \delta)$ is a bijection, but for now we describe, by example, how to obtain μ from a pair (τ, δ) in $P_n \times P_n$.

Example 9. Let $n = 8$, $\tau = (17)(45)(28)(36)$, and $\delta = (47)(15)(68)(23)$. We construct the orbit of 1 in μ by alternating applications τ and δ as follows:

$$\begin{array}{ll} \tau: & 1 \to 7, \\ \delta: & 7 \to 4, \\ \tau: & 4 \to 5, \\ \delta: & 5 \to 1. \end{array}$$

Thus the cycle of μ containing 1 is (1745). The next cycle begins with 2—the least element not in the first orbit. Again we follow the orbit of 2 by alternating applications of τ and δ:

$$\begin{array}{ll} \tau: & 2 \to 8, \\ \delta: & 8 \to 6, \\ \tau: & 6 \to 3, \\ \delta: & 3 \to 2. \end{array}$$

The cycle of μ containing 2 is (2863). In this way we recover all of the cycles of μ, and thus $\mu = (1745)(2863)$.

Denote the permutation $\mu \in E_n$ corresponding to $(\tau, \delta) \in P_n \times P_n$ by $\mu = \tau \times \delta$. Then the bijection between E_n and $P_n \times P_n$ is given by

$$\mu = \tau \times \delta \leftrightarrow (\tau, \delta).$$

We recap the discussion of this bijection and state two of its properties in the next lemma.

LEMMA 10. *The map* $\tau \times \delta \leftrightarrow (\tau, \delta)$ *is a bijection between* E_n *and* $P_n \times P_n$ *with the following properties*:

(i) $(\tau \times \delta)^{-1} = \delta \times \tau$, *and*
(ii) $\tau \times \tau = \tau$ *for all* τ, δ *in* P_n.

At last we can define the matrix $M(c)$. Order the elements of $P_n = \{\tau_1, \tau_2, \dots, \tau_N\}$. Then $M(c)$ is the N-by-N matrix given by

$$M(c) = \big(c(\tau_i \times \tau_j)\big).$$

Since the order of the elements in P_n is irrelevant, we will refer to the (τ, δ) entry $c(\tau \times \delta)$ of $M(c)$ without specifying the positions i, j where τ and δ appear in the list $\tau_1, \tau_2, \dots, \tau_N$.

At this point an example is appropriate. For $n = 4$,

$$P_4 = \{(12)(34), (13)(24), (14)(23)\}.$$

So $N = 3$, and for c a function on E_n, $M(c)$ is the 3-by-3 matrix

$$M(c) = \begin{bmatrix} c((12)(34)) & c((1243)) & c((1234)) \\ c((1342)) & c((13)(24)) & c((1324)) \\ c((1432)) & c((1423)) & c((14)(23)) \end{bmatrix}. \tag{8}$$

The $(1,3)$ entry, for example, is the value of c at $(12)(34) \times (14)(23) = (1234)$.

The next theorem gathers together a few facts about the matrix $M(c)$ when c is in the cone $\mathbf{C}_n$.

THEOREM 11. *Let* c *be in* $\mathbf{C}_n$. *Then* $M(c)$ *is a hermitian matrix with nonnegative diagonal entries.*

Now it is clear from Theorem 11 that we are interested only in the functions c on E_n for which $c(\tau \times \tau) \geqslant 0$ and

$$c(\tau \times \delta) = \overline{c(\delta \times \tau)},$$

for all $\tau, \delta \in P_n$. We denote the cone of all such functions by $\mathbf{E}_n^+$. In other words, $c \in \mathbf{E}_n^+$ if and only if $M(c)$ is hermitian with nonnegative diagonal entries. Theorem 11 says that $\mathbf{C}_n \subseteq \mathbf{E}_n^+$. But the reverse inclusion does not hold. For example, the matrix

$$M(c) = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

is hermitian and has nonnegative diagonal entries, but the only nonzero values of c are $c((1234)) = 1$ and $c((1432)) = 1$. Thus

$$d\left(c, \begin{bmatrix} 0 & -1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}\right) = -2,$$

so c is not in $\mathbf{C}_4$.

We now describe a condition on $M(c)$ (for $c \in \mathbf{E}_n^+$) that is sufficient to insure that $c \in \mathbf{C}_n$.

Let $B = (b_{ij})$ be an m-by-m complex matrix. Define the *comparison matrix* $\hat{B}$ of B by

$$\hat{B} = \begin{bmatrix} |b_{11}| & -|b_{12}| & \cdots & -|b_{1m}| \\ -|b_{21}| & |b_{22}| & \cdots & -|b_{2m}| \\ \vdots & \vdots & & \vdots \\ -|b_{m1}| & -|b_{m2}| & \cdots & |b_{mm}| \end{bmatrix}.$$

THEOREM 12. *Let c be a function in $\mathbf{E}_n^+$. Then $\hat{M}(c)$ is positive semidefinite if and only if c is a nonnegative linear combination of sparse functions. In particular, if $\hat{M}(c)$ is positive semidefinite, then $c \in \mathbf{C}_n$.*

For $n = 4$ we have a converse as well.

THEOREM 13. *Let c be a function in $\mathbf{E}_4^+$. Then $c \in \mathbf{C}_4$ if and only if $\hat{M}(c)$ is positive semidefinite.*

We should point out here that there are function $b \in \mathbf{C}_n$ for which $\hat{M}(b)$ is not positive semidefinite.

EXAMPLE 6 (REVISITED). The functions $b, c \in \mathbf{C}_8$ given in Example 6 are conjugates with nonzero values as follows:

$$c((12)(34)(56)(78)) = b((12)(34)(56)(78)) = 1,$$
$$c((1234)(5678)) = b((1234)(5876)) = \alpha,$$
$$c((1432)(5876)) = b((1432)(5678)) = \bar{\alpha},$$
$$c((23)(14)(58)(67)) = b((23)(14)(67)(58)) = |\alpha|^2.$$

The 4-by-4 principal submatrices of $M(c)$ and $M(b)$ (given below), lying in rows and columns (12)(34)(56)(78), (12)(34)(67)(85), (23)(41)(56)(78), (23)(41)(67)(85), contain all four nonzero entries in $M(c)$ and in $M(b)$:

$$\begin{bmatrix} 1 & 0 & 0 & \alpha \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \bar{\alpha} & 0 & 0 & |\alpha|^2 \end{bmatrix}, \qquad \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & \alpha & 0 \\ 0 & \bar{\alpha} & 0 & 0 \\ 0 & 0 & 0 & |\alpha|^2 \end{bmatrix}.$$

Thus $M(b)$ and $\hat{M}(b)$ are indefinite if α is nonzero, whereas $M(c)$ and $\hat{M}(c)$ are positive semidefinite.

Although a function c in $\mathbf{E}_n^+$ is completely determined by its associated matrix $M(c)$, there are many different functions c in $\mathbf{E}_n^+$ with the same associated comparison matrix $\hat{M}(c)$. Indeed, if $b, c \in \mathbf{E}_n^+$, then $|b(\mu)| = |c(\mu)|$ for all $\mu \in \mathbf{E}_n$ if and only if $\hat{M}(c) = \hat{M}(b)$. Among all functions $b \in \mathbf{E}_n^+$ satisfying $\hat{M}(b) = \hat{M}(c)$, we single out $\hat{c}$ defined for all $\tau \times \delta \in P_n \times P_n = E_n$ by

$$\hat{c}(\tau \times \delta) = -|c(\tau \times \delta)| \qquad \text{if} \quad \tau \neq \delta$$

and

$$\hat{c}(\tau \times \tau) = c(\tau \times \tau).$$

Then $M(\hat{c}) = \hat{M}(c)$, and the last part of Theorem 12 can be restated as follows: if $c \in \mathbf{E}_n^+$ and $M(\hat{c})$ is positive semidefinite, then $c \in \mathbf{C}_n$. Actually there is a simple inequality involving the generalized matrix functions $d(c, \cdot)$ and $d(\hat{c}, \cdot)$ that permits us to make a stronger statement.

THEOREM 14. *Let c be a function in $\mathbf{E}_n^+$ (not necessarily in $\mathbf{C}_n$), and let $A = (a_{ij})$ be in H_n. Then*

$$d(c, A) \geqslant d(\hat{c}, |A|),$$

where $|A| = (|a_{ij}|)$.

Now since $|A|$ is hermitian (actually symmetric) whenever A is hermitian, we have the following corollary to Theorem 14.

COROLLARY 15. *If* $\hat{c} \in \mathbf{C}_n$ *then* $c \in \mathbf{C}_n$.

Since $\hat{M}(c) = M(\hat{c}) = \hat{M}(\hat{c})$, Theorem 13 gives $\hat{c} \in \mathbf{C}_4$ if and only if $c \in \mathbf{C}_4$. Thus, it is tempting to conjecture that $\hat{c} \in \mathbf{C}_n$ if and only if $c \in \mathbf{C}_n$, for $n \geqslant 6$. But Example 16 is a counterexample.

EXAMPLE 16. Let b be the sparse function in $\mathbf{C}_4$ from Example 2, where $\alpha = 1$. Then from (8)

$$M(b) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{bmatrix}.$$

Let $c = b \otimes b$. From Theorems 3 and 7, $c \in \mathbf{C}_8$. But the only nonzero entries in $M(c)$ are ones lying in a 4-by-4 principal submatrix corresponding to rows (and columns) (12)(34)(56)(78), (12)(34)(67)(85), (23)(41)(56)(78), (23)(41)(67)(85). Thus the 4-by-4 principal submatrix of $\hat{M}(c)$ lying in the same rows (and columns) is

$$\begin{bmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{bmatrix}.$$

Now $\hat{c}(\sigma)$ equals 1 for four permutations σ, equals -1 for twelve permutations σ, and equals 0 for all other permutations σ in E_8. Let A be the matrix in H_8, all of whose entries are 1. Then $d(\hat{c}, A) = 4 - 12 < 0$, and so $\hat{c}$ is not in $\mathbf{C}_8$.

PROOFS

We begin with the proofs of the most technical results—Lemma 8, Lemma 10, Theorem 11, and an additional lemma (Lemma 17), which is needed to prove Theorem 11.

LEMMA 17. *Let c be a complex-valued function on* S_n. *Then*

(i) $d(c, A) = 0$ *for all* $A \in H_n$ *implies* $c \equiv 0$, *and*
(ii) $d(c, A)$ *real for all* $A \in H_n$ *implies* $c(\sigma^{-1}) = \overline{c(\sigma)}$ *for all* $\sigma \in S_n$.

Proof of Lemma 17. The proof of part (i) is an induction on n, so suppose that $d(c,\cdot)\equiv 0$ on H_m implies $c\equiv 0$ on S_m whenever $m<n$. Suppose c is a function on S_n and $d(c,\cdot)\equiv 0$ on H_n. Let σ be any permutation in S_n. We show that $c(\sigma)=0$. Now pick a cycle of σ. By replacing σ with $\phi\sigma\phi^{-1}$ (for an appropriate ϕ) and c with b [defined in (6)], we may assume that the cycle is $(1,2,\ldots,p)$. [$d(c,\cdot)\equiv 0$ implies $d(b,\cdot)\equiv 0$.] Thus $\sigma\in S_p\times S_q$, where $p+q=n$ and $S_p\times S_q$ is embedded in S_n in the usual way. So we write $\sigma=((1,2,\ldots,p),\ \delta)$ for some $\delta\in S_q$. If $q=0$, then $\sigma=(1,2,\ldots,n)$, and we will argue this case later. For now assume that $q>0$.

The next step is to define some function on S_q (either one, two, or four functions, depending on p), on which to use the inductive hypothesis. So for each $\pi\in S_q$ define

$$\begin{aligned} f(\pi) &= c((1,2,\ldots,p),\pi),\\ g(\pi) &= c((p,\ldots,2,1),\pi). \end{aligned} \tag{9}$$

If p is even, we need two more functions

$$\begin{aligned} h(\pi) &= c((12)(34)\cdots(p-1,p),\pi),\\ k(\pi) &= c((23)(45)\cdots(p,1),\pi). \end{aligned} \tag{10}$$

(If $p=2$, then the four functions f, g, h, k are identical.) We will show that $d(f,\cdot)\equiv 0$ if $p=2$; $d(f,\cdot)\equiv d(g,\cdot)\equiv 0$ if $p>2$ and p is odd; and $d(f,\cdot)\equiv d(g,\cdot)\equiv d(h,\cdot)\equiv d(k,\cdot)\equiv 0$ if $p>2$ and p is even. In any case the inductive hypothesis will imply that $f\equiv 0$ on S_q. Then, since $c(\sigma)=c(1,2,\ldots,p),\ \delta)=f(\delta)$, we shall have the desired result: $c(\sigma)=0$.

First we deal with the case $p=2$. Let

$$U=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}.$$

Now let $X\in H_q$. Since $U\oplus X\in H_n$, we have $0=d(c,U\oplus X)=d(f,X)$. Thus $d(f,\cdot)\equiv 0$ on H_q and by the induction hypothesis $f\equiv 0$. Hence $0=f(\delta)=c(\sigma)$.

The argument when $p>2$ is essentially the same as it is for $p=2$, but it requires a more complicated matrix to play the role of U. So for each pair of complex numbers x, y, define a p-by-p matrix in H_p by

$$U(p;x,y) = \begin{bmatrix} 0 & x & 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ \bar{x} & 0 & \bar{y} & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & y & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & & & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & & & & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & \cdot & 1 & 0 & 1 \\ 1 & 0 & \cdot & \cdot & \cdot & \cdot & 0 & 1 & 0 \end{bmatrix}. \tag{11}$$

The (i,j) entry of $U(p;\,x,\,y)$ is nonzero if and only if $j \equiv i \pm 1 \pmod p$. All of the nonzero entries are 1 except for x in position $(1,2)$, $\bar{x}$ in position $(2,1)$, $\bar{y}$ in position $(2,3)$, and y in position $(3,2)$. If p is odd, then $U(p;\,x,\,y)$ has only two nonzero diagonal products:

$$\begin{aligned} \Pi((1,2,\ldots,p),U(p;\,x,\,y)) &= x\bar{y}, \\ \Pi((p,\ldots,2,1),U(p;\,x,\,y)) &= \bar{x}y. \end{aligned} \tag{12}$$

If p is even, then $U(p;\,x,\,y)$ has two more nonzero diagonal products:

$$\begin{aligned} \Pi((12)(34)\cdots(p-1,p),U(p;\,x,\,y)) &= |x|^2, \\ \Pi((23)(45)\cdots(p,1),U(p;\,x,\,y)) &= |y|^2. \end{aligned} \tag{13}$$

Now let $X \in H_q$ and $A = U(p;\,x,\,y) \oplus X$. Then $A \in H_n$. Every nonzero diagonal product of A must be the product of a nonzero diagonal product of $U(p;\,x,\,y)$ and a diagonal product of X. Thus, from Equations (9), (10), (12) and (13), we have

$$0 = d(c,\,A) = x\bar{y}\,d(f,\,X) + \bar{x}y\,d(g,\,X) \tag{14}$$

if p is odd, and

$$\begin{aligned} 0 = d(c,\,A) &= |x|^2 d(h,\,X) + x\bar{y}\,d(f,\,X) \\ &\quad + \bar{x}y\,d(g,\,X) + |y|^2 d(k,\,X) \end{aligned} \tag{15}$$

if p is even. Since (14) and (15) hold for all choices of complex x, y it follows that $d(f,\cdot) \equiv d(g,\cdot) \equiv d(h,\cdot) \equiv d(k,\cdot) \equiv 0$ on H_q, which implies (by the induction hypothesis) that $f \equiv g \equiv h \equiv k \equiv 0$ on S_q. Thus $c(\sigma) = f(\delta) = 0$. This completes the proof of part (i) when $q > 0$.

It remains to show that $c(\sigma) = 0$ in case $q = 0$, i.e., when $\sigma = (1, 2, \ldots, n)$. This time let $A = U(n; x, y) \in H_n$. Then for all complex x, y,

$$0 = d(c, A) = x\bar{y}\, c(\sigma) + \bar{x}y\, c(\sigma^{-1})$$

if n is odd, and

$$0 = d(c, A) = |x|^2 c(\tau) + x\bar{y}\, c(\sigma) + \bar{x}y\, c(\sigma^{-1}) + |y|^2 c(\delta)$$

if n is even. Here $\tau = (12)(34) \cdots (n-1, n)$ and $\delta = (23)(45) \cdots (n, 1)$. It follows that $c(\sigma) = 0$. This completes the proof of part (i).

The proof of part (ii) can be deduced from part (i). Suppose $d(c, A)$ is real for all $A \in H_n$. Define a function b on S_n by

$$b(\sigma) = \overline{c(\sigma^{-1})}$$

for all $\sigma \in S_n$. For $A = (a_{ij}) \in H_n$ and $\sigma \in S_n$, we have

$$\Pi(\sigma^{-1}, A) = \overline{\Pi(\sigma, A)}\,.$$

Thus

$$\begin{aligned} d(b, A) &= \sum_\sigma b(\sigma)\Pi(\sigma, A) \\ &= \sum_\sigma \overline{c(\sigma^{-1})}\,\Pi(\sigma, A) \\ &= \sum_\sigma \overline{c(\sigma)}\,\Pi(\sigma^{-1}, A) \\ &= \overline{d(c, A)} \\ &= d(c, A). \end{aligned}$$

[The last equality comes from the hypothesis that $d(c, A)$ is real.] Thus $d(b - c, A) \equiv 0$ on H_n, and by part (i), $b - c \equiv 0$. ■

Proof of Lemma 8. Suppose $c \in \mathbf{C}_n$, and let σ be a permutation on S_n with a cycle of odd length p. By replacing σ with $\phi\sigma\phi^{-1}$ (for an appropriate ϕ) and c with b [defined in (6)], we may assume that this cycle is $(1, 2, \ldots, p)$, so that $\sigma = ((1, 2, \ldots, p), \delta) \in S_p \times S_q$ for some δ in S_q. ($c \in \mathbf{C}_n$ implies $b \in \mathbf{C}_n$.) For now, assume $q > 0$, and define c' on S_n by

$$c'(\mu) = \begin{cases} c(\mu) & \text{if} \quad \mu \in S_p \times S_q, \\ 0 & \text{otherwise}. \end{cases}$$

If

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \in H_n,$$

where $A_{11} \in H_p$, $A_{22} \in H_q$, then $0 \leqslant d(c, A_{11} \oplus A_{22}) = d(c', A)$ and so $c' \in \mathbf{C}_n$. But $-A_{11}$ is also in H_p, so $0 \leqslant d(c, (-A_{11}) \oplus A_{22}) = (-1)^p d(c, A_{11} \oplus A_{22}) = -d(c', A)$, since p is odd. It follows that $d(c', \cdot) \equiv 0$ on H_n and thus, by Lemma 17, $c' \equiv 0$ on S_n. In particular $c(\sigma) = c'((1, 2, \ldots, p), \delta) = 0$.

Now if $q = 0$, so that $\sigma = (1, \ldots, n)$ with n odd, then $d(c, -A) = -d(c, A)$ for all $A \in H_n$. Hence $d(c, \cdot) \equiv 0$, and by Lemma 17, $c(\sigma) = 0$. ∎

Proof of Lemma 10. The map $\mu \to (\tau, \delta)$, from E_n onto $P_n \times P_n$, described in (1), (2), and (4) is clearly one-to-one. To prove it is onto, we show how to recover $\mu = \tau \times \delta \in E_n$ from $(\tau, \delta) \in P_n \times P_n$. So assume $(\tau, \delta) \in P_n \times P_n$. We get the cycles of μ (and hence we get μ itself) from (τ, δ) as follows: The cycle μ_1 containing 1 is given by

$$\begin{aligned} \mu_1 : 1 \to \tau(1) \to \delta\tau(1) \to \tau\delta\tau(1) \to \cdots \\ \to (\delta\tau)^k(1) \to \tau(\delta\tau)^k(1) \to \cdots . \end{aligned} \tag{16}$$

The sequence in (16) contains two types of terms—those of the form $(\delta\tau)^k(1)$ and those of the form $\tau(\delta\tau)^k(1)$. It is not possible for a term of one type to equal a term of the other type. If, for example, $\tau(\delta\tau)^p(1) = (\delta\tau)^q(1)$ and $p \leqslant q$, then $\tau(r) = (\delta\tau)^{q-p}(r)$, where $r = (\delta\tau)^p(1)$. Since τ is an involution, $r = \tau(\delta\tau)^{q-p}(r)$ and so r is a fixed point of $\tau(\delta\tau)^{q-p}$. But $\tau(\delta\tau)^{q-p}$ is a conjugate of either τ or δ (depending on the parity of $q - p$), and hence $\tau(\delta\tau)^{q-p}$ has no fixed point, since all of its cycles are of length 2.

Now it follows that the first duplication in the list (16) occurs where a term $(\delta\tau)^k(1) = 1$. Thus

$$\mu_1 = \left(1, \tau(1), \delta\tau(1), \cdots, \tau(\delta\tau)^{k-1}(1)\right)$$

is a cycle with even length $2k$.

To construct the next cycle μ_2 of μ, take the smallest integer i that does not occur in μ_1 and let

$$\mu_2 = \left(i, \tau(i), \delta\tau(i), \ldots, (\delta\tau)^u(i), \tau(\delta\tau)^u(i), \cdots\right).$$

None of the integers in this cycle is equal to an integer in the cycle μ_1, and, by the same sort of argument as before, μ_2 is a cycle of even length. In the same manner we construct a set $\mu_1, \mu_2, \ldots, \mu_s$ of disjoint cycles of even length.

Now let $\mu = \mu_1 \cdots \mu_s$. Then $\mu \in E_n$ and clearly $\mu \to (\tau, \delta)$. Thus the map $\mu \to (\tau, \delta)$ is a bijection.

Parts (i) and (ii) of Lemma 10 follow immediately from the definition of $\tau \times \delta$. ■

Proof of Theorem 11. Let $c \in \mathbf{C}_n$. The fact that $M(c)$ is hermitian, i.e.

$$c(\tau \times \delta) = \overline{c(\delta \times \tau)},$$

follows immediately from Lemmas 10(i) and 17(ii).

To show that $c(\tau \times \tau) \geqslant 0$ for all $\tau \in P_n$, we need another test matrix A —the permutation matrix corresponding to τ. Since τ is a product of disjoint transpositions, $A \in H_n$ and so $0 \leqslant d(c, A)$. But A has only one nonzero diagonal product $\Pi(\sigma, A)$, namely $\Pi(\tau, A) = 1$. Thus $0 \leqslant d(c, A) = c(\tau) = c(\tau \times \tau)$. ■

Proof of Theorem 3. Let τ, δ be permutations in P_n, and let α be a complex number. The sparse function c corresponding to $\mu = \tau \times \delta$ and α is defined by

$$c(\tau) = 1, \qquad c(\mu) = \alpha,$$
$$c(\mu^{-1}) = \bar{\alpha}, \qquad c(\delta) = |\alpha|^2.$$

Proof of (i): To show that $c \in \mathbf{C}_n$, let $A = (a_{ij}) \in H_n$. Then

$$d(c, A) = \Pi(\tau, A) + \alpha\Pi(\mu, A) + \bar{\alpha}\Pi(\mu^{-1}, A) + |\alpha|^2\Pi(\delta, A),$$

and we must show that $0 \leqslant d(c, A)$. Now suppose that μ is the product of the cycles of even length given in (1) and (2). For each cycle,

$$\mu_s = (i(s,1), i(s,2), \dots, i(s,l_s))$$

of μ, define two sets of ordered pairs:

$$V(s) = \{(i(s,1), i(s,2)), (i(s,3), i(s,4)), \dots, (i(s,l_s - 1), i(s,l_s))\}$$

and

$$W(s) = \{(i(s,2), i(s,3)), (i(s,4), i(s,5)), \dots, (i(s,l_s), i(s,1))\},$$

and two corresponding partial diagonals of A by

$$\Pi(V, A) = \prod_s \prod_{(i,j)\in V(s)} a_{ij}$$

and

$$\Pi(W, A) = \prod_s \prod_{(i,j)\in W(s)} a_{ij}.$$

Each of these partial diagonals involves exactly half $(n/2)$ of the entries in each of the four diagonals of A corresponding to τ, μ, μ^{-1}, and δ. In fact,

$$\Pi(\tau, A) = \Pi(V, A)\,\overline{\Pi(V, A)},$$

$$\Pi(\mu, A) = \Pi(V, A)\Pi(W, A),$$

$$\Pi(\mu^{-1}, A) = \overline{\Pi(V, A)}\;\overline{\Pi(W, A)},$$

$$\Pi(\delta, A) = \Pi(W, A)\,\overline{\Pi(W, A)}.$$

Now it is easy to see why $0 \leqslant d(c, A)$:

$$d(c, A) = |\Pi(V, A) + \overline{\alpha\Pi(W, A)}|^2.$$

Proof of (ii): Let c be the sparse function corresponding to α and μ. Assume μ has at most one cycle of length greater than two, say $\mu = \mu_1 \mu_2$

$\cdots \mu_s$, where μ_1 is the cycle of length greater than two (if there is one) and $\mu_2, \ldots, \mu_s$ are transpositions. Suppose $\mu = \tau \times \delta$ for $\tau, \delta \in P_n$. For convenience we will deal with the conjugate, b, of c defined by (6) with ϕ taken so that $\mu_1 = (\phi(1), \phi(2), \ldots, \phi(p))$, $\mu_2 = (\phi(p+1), \phi(p+2)), \ldots, \mu_s = (\phi(n-1), \phi(n))$, and so that $\phi(1)$ is the least element in the cycle μ_1. Then $\phi^{-1}\mu_1\phi = (1, 2, \ldots, p)$, $\phi^{-1}\mu_2\phi = (p+1, p+2), \ldots, \phi^{-1}\mu_s\phi = (n-1, n)$, $\phi^{-1}\tau\phi = (12)(34)\cdots(p-1, p)(p+1, p+2)\cdots(n-1, n)$, and $\phi^{-1}\delta\phi = (23)(45)\cdots(p, 1)(p+1, p+2)\cdots(n-1, n)$. Now by replacing c with b we may assume that c is the sparse function corresponding to $\mu = (1, 2, \ldots, p)(p+1, p+2)\cdots(n-1, n)$ and α. [Although the conjugate of a sparse function is not generally a sparse function, in this special case (where μ has only one cycle of length greater than two) the conjugate b is a sparse function.]

To prove that $\langle c \rangle$ is an extreme ray in $\mathbf{C}_n$, suppose $f \in \mathbf{C}_n$ and

$$0 \leqslant d(f, A) \leqslant d(c, A)$$

for all $A \in H_n$. We must show that $f \in \langle c \rangle$.

To begin with, $f(\sigma) = 0$ unless σ is one of the four permutations $\tau = (12)(34)\cdots(p-1, p)(p+1, p+2)\cdots(n-1, n)$, $\delta = (23)(45)\cdots(p, 1)(p+1, p+2)\cdots(n-1, n)$, $\mu = \tau \times \delta$, or $\mu^{-1} = \delta \times \tau$, on which c is nonzero. To see this, let $A = (a_{ij}) \in H_n$, and for each real number x define $A(x) \in H_n$ by

$$A(x) = \begin{cases} a_{ij} & \text{if } (i, j) \in S, \\ x a_{ij} & \text{otherwise}, \end{cases}$$

where $S = \{(1,2), (2,1), (2,3), (3,2), \ldots, (p-1, p), (p, p-1), (p, 1), (1, p), (p+1, p+2), (p+2, p+1), (p+3, p+4), (p+4, p+3), \ldots, (n-1, n), (n, n-1)\}$. (The matrix positions listed in S are precisely those corresponding to the nonzero entries in $Q + Q^T$, where Q is the permutation matrix corresponding to μ.) Each diagonal product $\Pi(\sigma, A(0)) = 0$ unless $\sigma = \tau, \delta, \mu$, or μ^{-1}. Thus the constant term of the polynomial $d(f, A(x))$ equals

$$\begin{aligned} d(f, A(0)) = {} & f(\tau)\Pi(\tau, A) + f(\mu)\Pi(\mu, A) \\ & + f(\mu^{-1})\Pi(\mu^{-1}, A) + f(\delta)\Pi(\delta, A). \end{aligned}$$

On the other hand, since $c(\sigma) = 0$ unless $\sigma = \tau, \delta, \mu, \mu^{-1}$, and the diagonals of $A(x)$ corresponding to τ, δ, μ, and μ^{-1} do not involve any entry of $A(x)$ containing an x, we have $d(c, A(x)) = d(c, A)$. So $d(c, A(x))$ is a constant polynomial. But $0 \leqslant d(f, A(x)) \leqslant d(c, A(x)) = d(x, A)$ for all real x. So the polynomial $d(f, A(x))$ is bounded, and hence

$$d(f, A(x)) = d(f, A(0))$$

is a constant polynomial. Now define a function f' on E_n by

$$f'(\sigma) = \begin{cases} 0 & \text{if} \quad \sigma = \tau, \mu, \mu^{-1}, \text{or } \delta, \\ f(\sigma) & \text{otherwise.} \end{cases}$$

Then $d(f', A(x)) = d(f, A(x)) - d(f, A(0)) = 0$ for all x. In particular, $0 = d(f', A(1)) = d(f', A)$ for all $A \in H_n$. Now from Lemma 17, $f' \equiv 0$ and so $f(\sigma) = 0$, unless $\sigma = \tau$, μ, μ^{-1}, or δ.

Next we show that $f \in \langle c \rangle$. Let $U(p; x, y)$ be the matrix defined in (11). $U(p; x, y)$ has only four nonzero diagonal products, which are given in (12) and (13). [Actually $U(p; x, y)$ has only one nonzero diagonal if $p = 2$.] Now let

$$B(x, y) = U(p; x, y) \oplus W \oplus \cdots \oplus W,$$

where

$$W = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

appears $(n - p)/2$ times in the direct sum. Since $B(x, y) \in H_n$ for all complex x, y, we have $0 \leqslant d(f, B(x, y)) \leqslant d(c, B(x, y))$. But $B(x, y)$ has only four nonzero diagonal products—those corresponding to the permutations τ, μ, μ^{-1}, and δ. So

$$\begin{aligned} 0 &\leqslant f(\tau)|x|^2 + f(\mu)x\bar{y} + f(\mu^{-1})\bar{x}y + f(\delta)|y|^2 \\ &\leqslant |x|^2 + \alpha x\bar{y} + \overline{\alpha x}\, y + |\alpha|^2|y|^2. \end{aligned}$$

The above inequality between two hermitian forms in x and y can be rewritten in terms of the matrices for the forms as follows:

$$0 \leqslant [x, y]\begin{bmatrix} f(\tau) & f(\mu) \\ f(\mu^{-1}) & f(\delta) \end{bmatrix}\begin{bmatrix} \bar{x} \\ \bar{y} \end{bmatrix} \leqslant [x, y]\begin{bmatrix} 1 & \alpha \\ \bar{\alpha} & |\alpha|^2 \end{bmatrix}\begin{bmatrix} \bar{x} \\ \bar{y} \end{bmatrix}.$$

Since the matrix

$$\begin{bmatrix} 1 & \alpha \\ \bar{\alpha} & |\alpha|^2 \end{bmatrix}$$

has rank one, it follows that

$$\begin{bmatrix} f(\tau) & f(\mu) \\ f(\mu^{-1}) & f(\delta) \end{bmatrix} = r\begin{bmatrix} 1 & \alpha \\ \bar{\alpha} & |\alpha|^2 \end{bmatrix}$$

for some real number $0 \leqslant r \leqslant 1$. Hence $f \in \langle c \rangle$. ■

Proof of Theorem 7. Suppose $c_1 \in \mathbf{C}_p$ and $c_2 \in \mathbf{C}_q$. Let $c = c_1 \otimes c_2$ be the funtion on S_{p+q} defined by $c(\delta, \mu) = c_1(\delta)c_2(\mu)$ for $(\delta, \mu) \in S_p \times S_q$, and $c(\sigma) = 0$ *for* $\sigma \notin S_p \times S_q$. Part (i) of Theorem 7 holds because

$$d(c, A) = d(c_1, A_{11})d(c_2, A_{22}) \geqslant 0$$

for all

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \in H_{p+q}.$$

To prove part (ii) of Theorem 7, suppose $f \in \mathbf{C}_{p+q}$ and that $0 \leqslant d(f, A) \leqslant d(c, A)$ for all $A \in H_{p+q}$. We must show that $f = rc$ for some real number $0 \leqslant r \leqslant 1$. First we show that $f(\sigma) = 0$ unless $\sigma \in S_p \times S_q$. Let

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad \text{and} \quad A(x) = \begin{bmatrix} A_{11} & xA_{12} \\ xA_{21} & A_{22} \end{bmatrix}.$$

Then for each real number x,

$$0 \leqslant d(f, A(x)) \leqslant d(c, A(x)) = d(c_1, A_{11})d(c_2, A_{22}).$$

So the polynomial $d(f, A(x))$ is bounded and hence is a constant polynomial, i.e., $d(f, A(x)) = d(f, A(0))$. Define a function f' on S_{p+q} by

$$f'(\sigma) = \begin{cases} 0 & \text{if} \quad \sigma \in S_p \times S_q, \\ f(\sigma) & \text{otherwise.} \end{cases}$$

Then $d(f', A(x)) = d(f, A(x)) - d(f, A(0)) = 0$. In particular, $0 = d(f', A(1)) = d(f', A)$ for all $A \in H_{p+q}$. So by Lemma 17, $f' \equiv 0$, and thus $f(\sigma) = 0$ unless $\sigma \in S_p \times S_q$.

Now we show that $f = rc$ for some real number $0 \leqslant r \leqslant 1$. Let $Y \in H_q$. Define a function g, which depends on Y, on S_p as follows: for $\mu \in S_p$, let

$$g(\mu) = \sum_{\delta \in S_q} f(\mu, \delta)\Pi(\delta, Y).$$

Now if $X \in H_p$, then

$$\begin{aligned} d(g, X) &= \sum_{\mu} g(\mu)\Pi(\mu, X) \\ &= \sum_{\mu, \delta} f(\mu, \delta)\Pi(\mu, X)\Pi(\delta, Y) \\ &= d(f, X \oplus Y) \\ &\leqslant d(c_1, X)d(c_2, Y). \end{aligned}$$

(The sums are taken over $\mu \in S_p$ and $\delta \in S_q$.) Thus $g \in \mathbf{C}_p$, and since $\langle c_1 \rangle$ is an extreme ray in $\mathbf{C}_p$, $g \in \langle c_1 \rangle$. So there is a nonnegative number $\Phi(Y)$ such that $g = \Phi(Y)c_1$. (Remember that g depends on the choice of Y in H_q.) It follows that

$$d(f, X \oplus Y) = \Phi(Y)d(c_1, X)$$

for all $X \in H_p$, $Y \in H_q$. Similarly, there is a function Γ on H_p such that

$$d(f, X \oplus Y) = \Gamma(X)d(c_2, Y) \tag{17}$$

for all $X \in H_p$, $Y \in H_q$. So we have

$$\Gamma(X)d(c_2, Y) = \Phi(Y)d(c_1, X) \tag{18}$$

for all $X \in H_p$, $Y \in H_q$.

Now the argument splits into two cases.

Case 1: $d(c_2, Y) = 0$ *for all* $Y \in H_q$. Then $c_2 \equiv 0$, $c = c_1 \otimes c_2 \equiv 0$, and since $d(f, X \oplus Y) = 0$ for all $X \in H_p$ and $Y \in H_q$, we have $f \equiv 0$. Hence $f \in \langle c \rangle$.

Case 2: $d(c_2, Y') > 0$ *for some* $Y' \in H_q$. Let $r = \Phi(Y')/d(c_2, Y')$; *then from* (18) *we have*

$$\Gamma(X) = rd(c_1, X)$$

for all $X \in H_p$. *Thus from* (17) *we have*

$$d(f, X \oplus Y) = rd(c_1, X)d(c_2, Y) = rd(c, X \oplus Y)$$

for all $X \in H_p$ and $Y \in H_q$. It follows from Lemma 17 that $f = rc$.

Conversely, suppose $c_1 \otimes c_2$ generates an extreme ray in $\mathbf{C}_{p+q}$. To show that c_1 generates an extreme ray in $\mathbf{C}_p$, suppose that $c_1 = a_1 + b_1$ with a_1, b_1 in $\mathbf{C}_p$. Then $c_1 \otimes c_2 = a_1 \otimes c_2 + b_1 \otimes c_2$. Since $c_1 \otimes c_2$ generates an extreme ray, $a_1 \otimes c_2 = r(c_1 \otimes c_2)$ for some $0 < r < 1$. It follows from $c_2 \not\equiv 0$ that $a_1 = rc_1$. So c_1 generates an extreme ray. ∎

Proof of Theorem 12. The first part of Theorem 12 follows from a more general result about the cone

$$K_m = \Big\{M = (m_{ij}) \in H_m : \hat{M} \text{ is positive semidefinite and } m_{ii} \geqslant 0,\ i = 1, \dots, m\Big\}.$$

It is clear that the ray $\langle M \rangle = \{rM : r \geqslant 0\}$ is in K_m whenever $M \in K_m$. But not so clear is the fact that K_m is a convex cone and that the sparse matrices generate this cone. (An m-by-m matrix M is *sparse* if its only nonzero entries are

$$m_{ii} = 1, \qquad m_{ij} = \alpha, \qquad m_{ji} = \bar{\alpha}, \qquad m_{jj} = |\alpha|^2$$

for some $i < j$ and complex number α.) Now if $c \in \mathbf{E}_n^+$, then $M(c)$ is a hermitian matrix with nonnegative diagonal and c is a nonnegative linear combination of sparse functions in $\mathbf{C}_n$ if and only if $M(c)$ is a nonnegative linear combination of sparse matrices. So the first part of Theorem 12 follows from this lemma:

LEMMA 18. *Let M be an m-by-m hermitian matrix. Then $M \in K_m$ if and only of M is a nonnegative linear combination of sparse matrices.*

Proof of Lemma 18. First we show that if $M \in K_m$, then M is a positive linear combination of sparse matrices. So assume $M \in K_m$. Then $\hat{M}$ is an

M-matrix, and it follows from [3, Theorem 4.1], for example, that there is a positive m-tuple v such that $\hat{M}v \geqslant 0$. (Each component of $\hat{M}v$ is nonnegative.) Now let D be the diagonal matrix whose (i, i) entry is the ith entry of v. Then the row sums of $\hat{M}D$ are nonnegative, which implies that the row sums of $D\hat{M}D$ are also nonnegative. (In other words, DMD is row diagonally dominant.)

Next we show that $DMD = M' = (m_{ij})$ is a nonnegative linear combination of sparse matrices of the form

$$E_{ii} + \zeta E_{ij} + \bar{\zeta} E_{ji} + E_{jj} \quad \text{and} \quad E_{ii},$$

where E_{st} is the matrix whose only nonzero entry is a 1 in position (s, t) and where ζ is a complex number with $|\zeta| = 1$. But

$$M' = \sum_{i<j} \left(|m_{ij}| E_{ii} + m_{ij} E_{ij} + \overline{m_{ij}} E_{ji} + |m_{ij}| E_{jj} \right) + \sum_{i} m_i E_{ii}, \tag{19}$$

where

$$m_i = m_{ii} - \sum_{j \neq i} |m_{ij}|,$$

and since M' is row diagonally dominant, $m_i \geqslant 0$ for $i = 1, \dots, m$. Each nonzero matrix in the first sum in (19) is of the form

$$r\left(E_{ii} + \zeta E_{ij} + \bar{\zeta} E_{ji} + E_{jj}\right),$$

where $r = |m_{ij}|$ and $\zeta = m_{ij}/|m_{ij}|$.

Now it follows that $M = D^{-1}M'D^{-1}$ is a nonnegative linear combination of matrices of the form

$$E_{ii} + \alpha E_{ij} + \bar{\alpha} E_{ji} + |\alpha|^2 E_{jj}. \tag{20}$$

(α can be zero.) Thus M is a nonnegative linear combination of sparse matrices.

Conversely, suppose M is a nonnegative linear combination of sparse matrices. A sparse matrix can have nonzero entries in only two off-diagonal positions—(i, j) and (j, i), for some $i < j$. Such a sparse matrix is said to be of *type* (i, j). All other sparse matrices have just one nonzero entry, and it is a 1 on the main diagonal.

Suppose M is a nonnegative linear combination

$$M = \sum_{i<j} b_{ij} S_{ij} + D, \tag{21}$$

where $b_{ij} \geqslant 0$, S_{ij} is a sparse matrix of type (i, j), and D is nonnegative diagonal matrix. Then

$$\hat{M} = \sum_{i<j} b_{ij} \hat{S}_{ij} + D$$

is positive semidefinite, since each $\hat{S}_{ij}$ is positive semidefinite. So if M is a positive linear combination of sparse matrices and for each $i < j$ there is only one sparse matrix of type (i, j) in the linear combination, then $M \in K_m$.

The more difficult case occurs when M is a nonnegative linear combination of sparse matrices and there is more than one nonzero sparse matrix of a given type in the linear combination. So we examine a positive linear combination of two sparse matrices of the same type, say type (i, j). Suppose the principal submatrices of those two sparse matrices lying in rows and columns i, j are

$$A = \begin{bmatrix} 1 & \alpha \\ \bar{\alpha} & |\alpha|^2 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 1 & \beta \\ \bar{\beta} & |\beta|^2 \end{bmatrix}.$$

Then the positive linear combination $aA + bB$ is a sum of positive scalar multiples of two other sparse matrices, one of which is a diagonal matrix, viz.,

$$aA + bB = (a + b)\left(\begin{bmatrix} 1 & a'\alpha + b'\beta \\ a'\bar{\alpha} + b'\bar{\beta} & |a'\alpha + b'\beta|^2 \end{bmatrix} + a'b'\begin{bmatrix} 0 & 0 \\ 0 & |\alpha - \beta|^2 \end{bmatrix}\right),$$

where $a' = a/(a + b)$ and $b' = b/(a + b)$. It follows that M is a nonnegative linear combination of sparse matrices in which there is only one sparse matrix of each type (i, j). So now M can be expressed as the sum in (21), and from the previous argument, $\hat{M}$ is positive semidefinite. ■

Proof of Theorem 13. Let $n = 4$, and let c be a function in $\mathbf{E}_4^+$. We already know from Theorem 12 that if $\hat{M}(c)$ is positive semidefinite, then $c \in \mathbf{C}_4$. It remains to prove the converse.

Suppose $c \in \mathbf{C}_4$, and let

$$M(c) = \begin{bmatrix} r & \beta & \alpha \\ \bar{\beta} & s & \gamma \\ \bar{\alpha} & \bar{\gamma} & t \end{bmatrix},$$

where r, s, t are nonnegative. We must show that

$$\hat{M}(c) = \begin{bmatrix} r & -|\beta| & -|\alpha| \\ -|\beta| & s & -|\gamma| \\ -|\alpha| & -|\gamma| & t \end{bmatrix}$$

is positive semidefinite. To do this let

$$A = \begin{bmatrix} 0 & x_1 & x_2 & x_3 \\ \overline{x_1} & 0 & u & v \\ \overline{x_2} & \bar{u} & 0 & w \\ \overline{x_3} & \bar{v} & \bar{w} & 0 \end{bmatrix}.$$

Then for any choice of complex numbers x_1, x_2, x_3, u, v, w, the matrix A is in H_4. Now $d(c, A)$ is a (quadratic) hermitian form in x_1, x_2, x_3 with coefficients involving $u, v, w, r, s, t, \alpha, \beta, \gamma$. A direct calculation shows that $d(c, A) = xM(u, v, w)x*$, where $x = (x_1, x_2, x_3)$, $x*$ is the conjugate transpose of x, and

$$M(u,v,w) = \begin{bmatrix} rw\bar{w} & \beta v\bar{w} & \alpha uw \\ \bar{\beta}\bar{v}w & sv\bar{v} & \gamma v\bar{u} \\ \overline{\alpha uw} & \overline{\gamma v u} & tu\bar{u} \end{bmatrix}.$$

Since $d(c, A) \geqslant 0$, the matrix $M(u, v, w)$ is positive semidefinite for all choices of u, v, w.

To show that $\hat{M}(c)$ is positive semidefinite, we find complex numbers u, v, w such that $M(u, v, w) = \hat{M}(c)$. To this end write the complex numbers $\alpha = |\alpha|\omega$, $\beta = |\beta|\zeta$, and $\gamma = |\gamma|\tau$ in polar form so that $|\omega| = |\zeta| = |\tau| = 1$. Let

$$\theta = \sqrt{-\ \overline{\zeta\omega\tau}}\ .$$

Now pick

$$u = \overline{\omega\zeta\theta}\,, v = \theta, w = -\zeta\theta.$$

Then

$$M\left(\overline{\omega\zeta\theta}, \theta, -\zeta\theta\right) = \hat{M}(c)$$

is positive semidefinite. ■

Proof of Theorem 4. Let c be a function in $\mathbf{C}_4$. From Theorem 13, $\hat{M}(c)$ is positive semidefinite and thus, by Theorem 12, c is a positive linear combination of sparse functions. ■

Proof of Theorem 14. Let c be a function in $\mathbf{E}_n^+$ and let A be in H_n. Then

$$\begin{aligned} d(c, A) &= \sum_{\tau} c(\tau)\Pi(\tau, A) \\ &\quad + \sum_{\tau \neq \delta} c(\tau \times \delta)\Pi(\tau \times \delta, A) \\ &\geqslant \sum_{\tau} c(\tau)\Pi(\tau, A) \\ &\quad - \sum_{\tau \neq \delta} |c(\tau \times \delta)||\Pi(\tau \times \delta, A)|, \end{aligned}$$

where the sums are taken over τ, δ in P_n. But

$$|\Pi(\tau \times \delta, A)| = \Pi(\tau \times \delta, |A|),$$

and

$$\Pi(\tau, A) = \Pi(\tau, |A|).$$

Thus

$$\begin{aligned} d(c, A) &\geqslant \sum_{\tau} c(\tau)\Pi(\tau, |A|) - \sum_{\tau \neq \delta} |c(\tau \times \delta)|\Pi(\tau \times \delta, |A|) \\ &= \sum_{\tau} \hat{c}(\tau)\Pi(\tau, |A|) + \sum_{\tau \neq \delta} \hat{c}(\tau \times \delta)\Pi(\tau \times \delta, |A|) \\ &= d(\hat{c}, |A|). \end{aligned}$$

■

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